```
=> s l9 and l8
L10             3 L9 AND L8

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     2.36     317.45

FILE 'REGISTRY' ENTERED AT 23:00:15 ON 07 NOV 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     5 NOV 2004  HIGHEST RN 775356-23-5
DICTIONARY FILE UPDATES:    5 NOV 2004  HIGHEST RN 775356-23-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L11      STRUCTURE UPLOADED

=>  l11
L11 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d l11
L11 HAS NO ANSWERS
L11              STR
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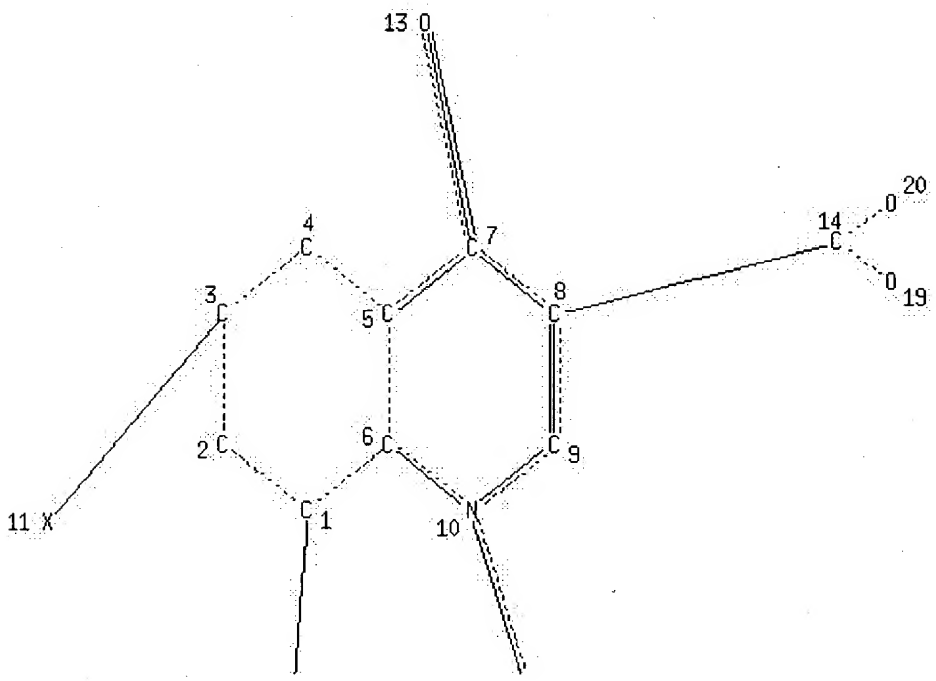
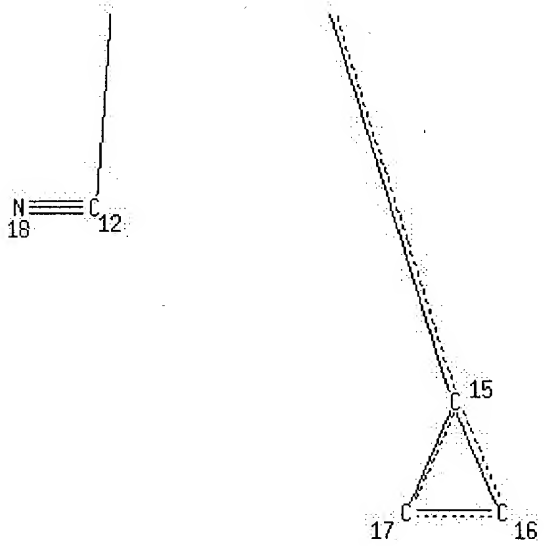


Page 1-A



Page 2-A

NODE ATTRIBUTES:

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NSPEC	IS R	AT	4
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NSPEC	IS C	AT	11
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NSPEC	IS C	AT	14
NSPEC	IS R	AT	15

h eb c g cg b cg eb

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NSPEC   IS R      AT  16
NSPEC   IS R      AT  17
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS C      AT  20
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  11 12 13 14 18 19 20
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   1
NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE


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SAMPLE SEARCH INITIATED 23:02:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      6 TO ITERATE

100.0% PROCESSED       6 ITERATIONS                              4 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            6 TO      266
PROJECTED ANSWERS:               4 TO      200

L12           4 SEA SSS SAM L11

=> s l11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 23:02:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     89 TO ITERATE

100.0% PROCESSED      89 ITERATIONS                             48 ANSWERS
SEARCH TIME: 00.00.01

L13          48 SEA SSS FUL L11

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             156.26     473.71

FILE 'HCAPLUS' ENTERED AT 23:02:20 ON 07 NOV 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
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h eb c g cg b cg eb

FILE COVERS 1907 - 7 Nov 2004 VOL 141 ISS 20
FILE LAST UPDATED: 6 Nov 2004 (20041106/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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FILE 'REGISTRY' ENTERED AT 22:56:32 ON 07 NOV 2004
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L2 2 S L1
L3 23 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:58:20 ON 07 NOV 2004
L4 12 S L3

FILE 'REGISTRY' ENTERED AT 22:58:25 ON 07 NOV 2004
L5 STRUCTURE UPLOADED
L6 0 S L5
L7 19 S L5 FULL

FILE 'HCAPLUS' ENTERED AT 22:59:56 ON 07 NOV 2004
L8 31 S L7/RCT
L9 4 S L3/PREP
L10 3 S L9 AND L8

FILE 'REGISTRY' ENTERED AT 23:00:15 ON 07 NOV 2004
L11 STRUCTURE UPLOADED
L12 4 S L11
L13 48 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 23:02:20 ON 07 NOV 2004

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24 L13
2674061 RCT/RL
L14 8 L13/RCT
(L13 (L) RCT/RL)

=> d his

(FILE 'HOME' ENTERED AT 22:56:26 ON 07 NOV 2004)

FILE 'REGISTRY' ENTERED AT 22:56:32 ON 07 NOV 2004
L1 STRUCTURE UPLOADED
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L3 23 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:58:20 ON 07 NOV 2004
L4 12 S L3

FILE 'REGISTRY' ENTERED AT 22:58:25 ON 07 NOV 2004
L5 STRUCTURE UPLOADED
L6 0 S L5
L7 19 S L5 FULL

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     FILE 'HCAPLUS' ENTERED AT 22:59:56 ON 07 NOV 2004
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L9             4 S L3/PREP
L10            3 S L9 AND L8

     FILE 'REGISTRY' ENTERED AT 23:00:15 ON 07 NOV 2004
L11              STRUCTURE UPLOADED
L12            4 S L11
L13           48 S L11 FULL

     FILE 'HCAPLUS' ENTERED AT 23:02:20 ON 07 NOV 2004
L14            8 S L13/RCT

=> s l14 and l10
L15            3 L14 AND L10

=> d l15, ibib abs hitstr, 1-3

L15  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

ACCESSION NUMBER: 2000:366037 HCAPLUS
DOCUMENT NUMBER: 133:4647
TITLE: Semihydrochloride of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): Himmler, Thomas; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854357	A1	20000531	DE 1998-19854357	19981125
CA 2351714	AA	20000602	CA 1999-2351714	19991115
WO 2000031077	A1	20000602	WO 1999-EP8778	19991115
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1133495	A1	20010919	EP 1999-955995	19991115
EP 1133495	B1	20021009		
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JP 2002530408	T2	20020917	JP 2000-583905	19991115
AT 225790	E	20021015	AT 1999-955995	19991115
ES 2181488	T3	20030216	ES 1999-955995	19991115
PT 1133495	T	20030228	PT 1999-955995	19991115

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AU 759769	B2	20030501	AU 2000-12716		19991115
NZ 511863	A	20030530	NZ 1999-511863		19991115
NO 2001002532	A	20010702	NO 2001-2532		20010523
PRIORITY APPLN. INFO.:			DE 1998-19854357	A	19981125
			WO 1999-EP8778	W	19991115

OTHER SOURCE(S): CASREACT 133:4647
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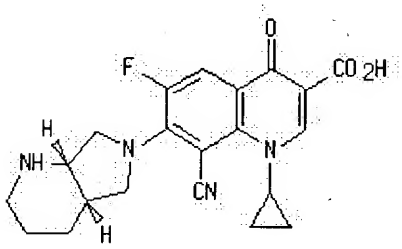


I

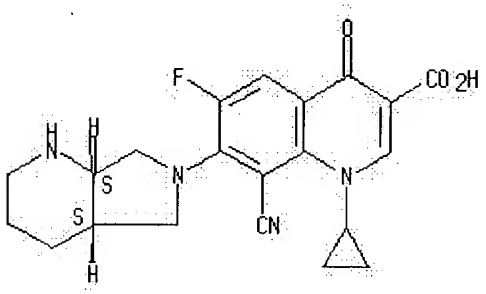
AB The title compd. (I), useful as a medical and veterinary bactericide, shows good water soly. (19 wt.%). I is produced by reaction of 7-halo-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid with (1S,6S)-2,8-diazabicyclo[4.3.0]nonane in the presence of a base in one of the following diluents: (a) a C≥4 aliph. alc., (b) a mixt. of a C>3 alc. with the polar aprotic diluent, N-methylpyrrolidone; (c) a mixt. of n-PrOH with DMF. I (m. 278-280°) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

IT **271252-05-2P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**; PROC (Process)
(semihydrochloride of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 271252-05-2 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, hydrochloride (2:1) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



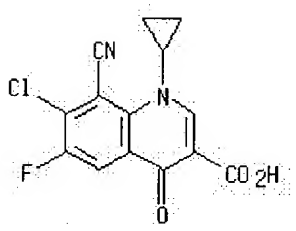
1/2 HCl

IT **117528-65-1**, 7-Chloro-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid **151213-40-0**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(semihydrochloride of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 117528-65-1 HCAPLUS

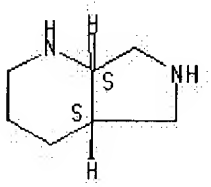
h eb c g cg b cg eb

CN 3-Quinolinecarboxylic acid, 7-chloro-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



RN 151213-40-0 HCAPLUS
CN 1H-Pyrrolo[3,4-b]pyridine, octahydro-, (4aS,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L15 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:366035 HCAPLUS
DOCUMENT NUMBER: 133:4645
TITLE: Crystal modification B of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): Himmler, Thomas; Hallenbach, Werner; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854355	A1	20000531	DE 1998-19854355	19981125
CA 2351707	AA	20000602	CA 1999-2351707	19991115
WO 2000031076	A1	20000602	WO 1999-EP8776	19991115
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1133497	A1	20010919	EP 1999-959278	19991115
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JP 2002530407	T2	20020917	JP 2000-583904		19991115
NZ 511862	A	20030829	NZ 1999-511862		19991115
AU 767890	B2	20031127	AU 2000-16517		19991115
NO 2001002461	A	20010518	NO 2001-2461		20010518
US 6664268	B1	20031216	US 2001-856670		20010523
PRIORITY APPLN. INFO.:			DE 1998-19854355	A	19981125
			WO 1999-EP8776	W	19991115

OTHER SOURCE(S): CASREACT 133:4645

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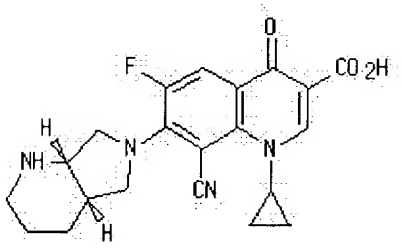


I

AB The title compd. in crystal modification B (I), useful as a medical and veterinary bactericide, is stable during extended storage without conversion to the amorphous form or any other crystal modification, and is less hygroscopic than the amorphous form of the compd. I is produced either (a) by reaction of 7-halo-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid with (1S,6S)-2,8-diazabicyclo[4.3.0]nonane in the presence of a base in a mixt. of EtOH and a polar aprotic diluent such as N-methylpyrrolidone, DMF, or sulfolane, or (b) by heating an unknown modification of the compd. in the presence of a base in EtOH, n-PrOH, iso-PrOH, or a mixt. of one of these alcs. with one of the polar aprotic diluents named previously. I (m. 243-245°) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

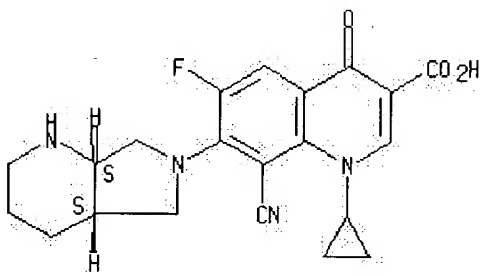
IT **195532-12-8P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**; PROC (Process)
(crystal modification B of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

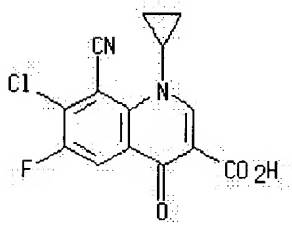


IT **117528-65-1**, 7-Chloro-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid **151213-40-0**

RL: **RCT (Reactant)**; RACT (Reactant or reagent)

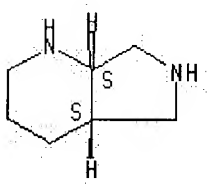
h eb c g cg b cg eb

(crystal modification B of cyanocyclopropyl(diazabicyclononyl)fluorodih
ydrooxoquinolinecarboxylic acid)
RN 117528-65-1 HCAPLUS
CN 3-Quinolinecarboxylic acid, 7-chloro-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



RN 151213-40-0 HCAPLUS
CN 1H-Pyrrolo[3,4-b]pyridine, octahydro-, (4aS,7aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L15 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 1997:579724 HCAPLUS
DOCUMENT NUMBER: 127:248093
TITLE: 8-Cyano-1-cyclopropyl-7-(2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid derivatives
INVENTOR(S): Bartel, Stefan; Jaetsch, Thomas; Himmler, Thomas; Rast, Hans-Georg; Hallenbach, Werner; Heinen, Ernst; Pirro, Franz; Scheer, Martin; Stegemann, Michael; Stupp, Hans-Peter; Wetzstein, Heinz-Georg
PATENT ASSIGNEE(S): Bayer A.-G., Germany; Bartel, Stefan; Jaetsch, Thomas; Himmler, Thomas; Rast, Hans-Georg; Hallenbach, Werner; Heinen, Ernst; Pirro, Franz; Scheer, Martin; et al.
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9731001	A1	19970828	WO 1997-EP637	19970212
W: AU, BB, BG, BR, BY, CA, CN, CZ, HU, IL, JP, KR, KZ, LK, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19633805	A1	19970828	DE 1996-19633805	19960822
ZA 9701507	A	19970916	ZA 1997-1507	19970202
CA 2247020	AA	19970828	CA 1997-2247020	19970212
AU 9717689	A1	19970910	AU 1997-17689	19970212

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AU 715341	B2	20000120		
EP 882049	A1	19981209	EP 1997-903260	19970212
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CN 1073112	B	20011017		
BR 9707606	A	19990727	BR 1997-7606	19970212
NZ 331468	A	20000228	NZ 1997-331468	19970212
JP 2000504734	T2	20000418	JP 1997-529755	19970212
IL 125444	A1	20010319	IL 1997-125444	19970212
RU 2173318	C2	20010910	RU 1998-117814	19970212
EP 1215202	A1	20020619	EP 2002-6519	19970212
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ES 2184060	T3	20030401	ES 1997-903260	19970212
PT 882049	T	20030430	PT 1997-903260	19970212
PL 186737	B1	20040227	PL 1997-328577	19970212
TW 390879	B	20000521	TW 1997-86101994	19970220
US 6323213	B1	20011127	US 1998-125191	19980813
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CN 1335301	A	20020213	CN 2001-110855	20010228
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OTHER SOURCE(S): MARPAT 127:248093

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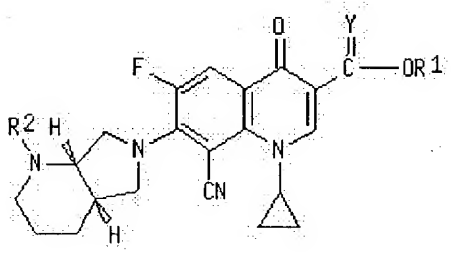


I

AB Title compds. I [R1 = H, alkyl, optionally substituted by OH, OMe, NH2, NHMe, NMe2, or (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl; R2 = H, benzyl, alkyl, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl, CH=CHCO2R3, CH2CH2CO2R3, CH2CH2CN, CH2CH2COMe, CH2COMe; R3 = Me, Et, R4(NHCHR5CO)n; R4 = H, alkyl, CO2CMe3; R5 = H, alkyl, hydroxyalkyl, aminoalkyl, thioalkyl, carboxyalkyl, benzyl; n = 1, 2; Y = O, S] were prepd. for use as antibacterial agents. Thus, I [R1 = OH, R2 = H, Y = O] was prepd. by aminating the 7-chloroquinoline. I [R1 = OH, R2 = H, Y = O] had min. inhibitory concns. against a no. of bacteria that were superior to those of enrofloxacin.

IT **195532-12-8P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(prepn. of diazabicylononylquinolinecarboxylic acid derivs. as bactericides)

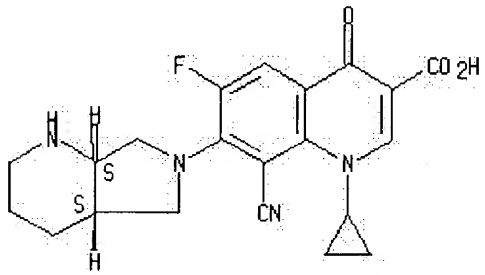
RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-

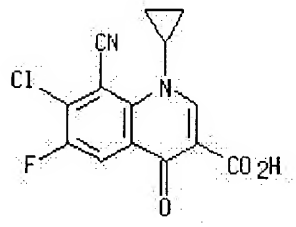
h eb c g cg b cg eb

[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

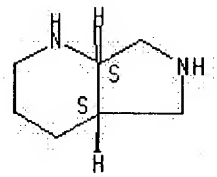


IT 117528-65-1 151213-40-0
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of diazabicylononylquinolinecarboxylic acid derivs. as bactericides)
RN 117528-65-1 HCAPLUS
CN 3-Quinolinecarboxylic acid, 7-chloro-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)



RN 151213-40-0 HCAPLUS
CN 1H-Pyrrolo[3,4-b]pyridine, octahydro-, (4aS,7aS)- (9CI) (CA INDEX NAME)

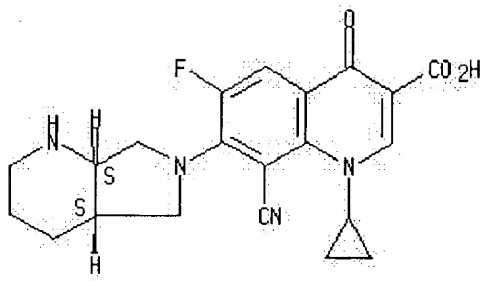
Absolute stereochemistry. Rotation (-).



IT **195532-14-0P** **195532-16-2P** **195532-18-4P**
195532-20-8P **195532-22-0P** **195532-25-3P**
195532-27-5P **195532-29-7P** **195532-31-1P**
195532-33-3P **195532-36-6P** **195532-39-9P**
195532-42-4P **195532-45-7P** **195532-48-0P**
195532-58-2P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of diazabicylononylquinolinecarboxylic acid derivs. as bactericides)
RN 195532-14-0 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

h eb c g cg b cg eb



HCl

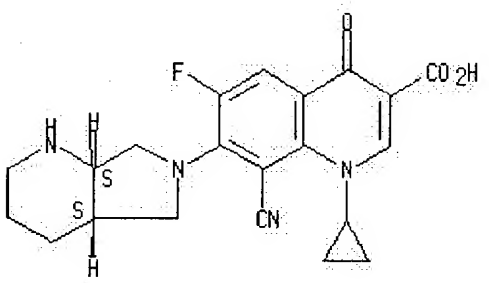
RN 195532-16-2 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

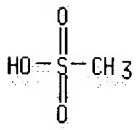
CRN 195532-12-8
CMF C21 H21 F N4 O3

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 195532-18-4 HCAPLUS

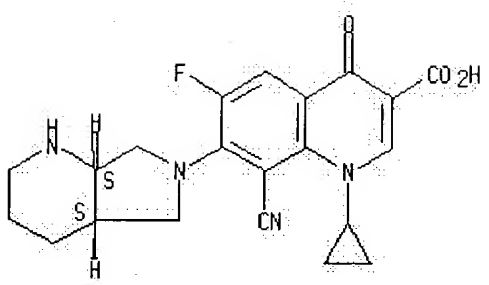
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 195532-12-8
CMF C21 H21 F N4 O3

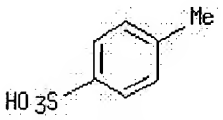
Absolute stereochemistry.

h eb c g cg b cg eb



CM 2

CRN 104-15-4
CMF C7 H8 O3 S

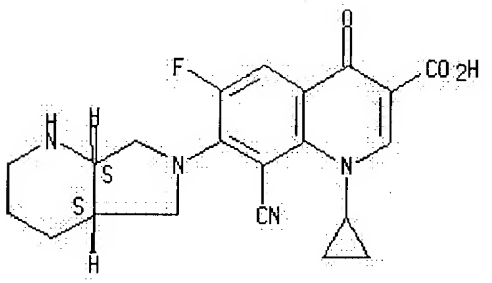


RN 195532-20-8 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

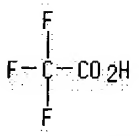
CRN 195532-12-8
CMF C21 H21 F N4 O3

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

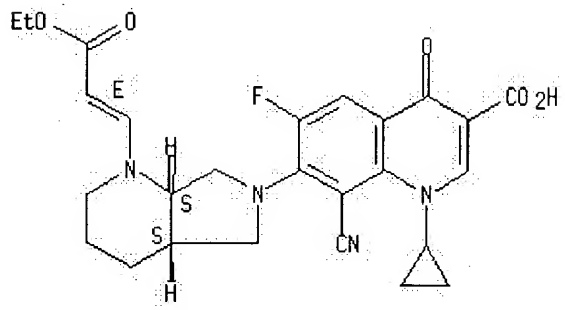


RN 195532-22-0 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-7-[1-(3-ethoxy-3-oxo-1-propenyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-6-fluoro-1,4-dihydro-4-oxo-, [4aS-[1(E),4aα,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

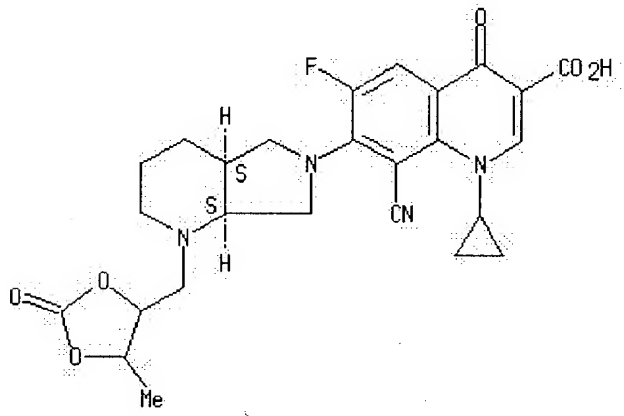
h eb c g cg b cg eb

Double bond geometry as shown.



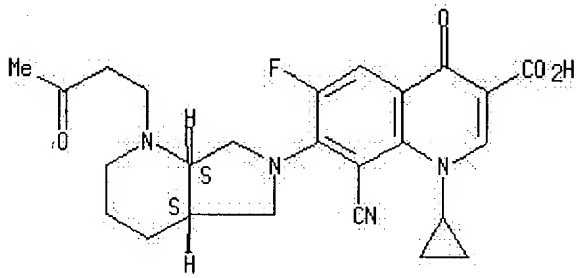
RN 195532-25-3 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[octahydro-1-[(5-methyl-2-oxo-1,3-dioxolan-4-yl)methyl]-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, [4aS-(4aα,7aα)]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 195532-27-5 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[octahydro-1-(3-oxobutyl)-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

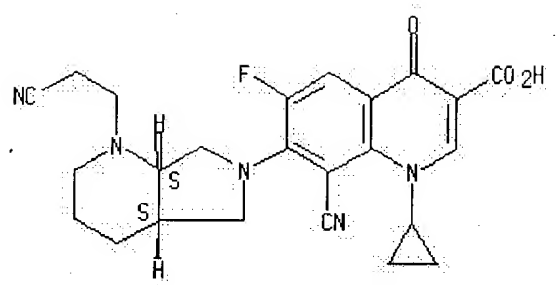
Absolute stereochemistry.



RN 195532-29-7 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-7-[1-(2-cyanoethyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

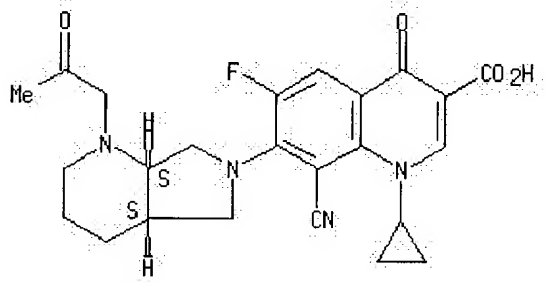
Absolute stereochemistry.

h eb c g cg b cg eb



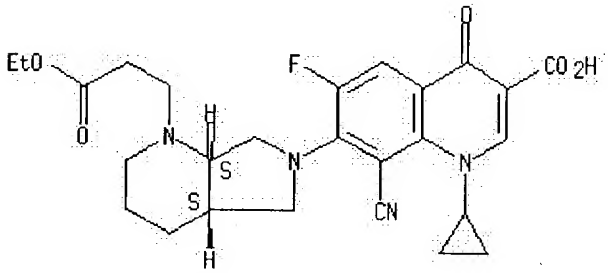
RN 195532-31-1 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[octahydro-1-(2-oxopropyl)-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 195532-33-3 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-7-[1-(3-ethoxy-3-oxopropyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-6-fluoro-1,4-dihydro-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

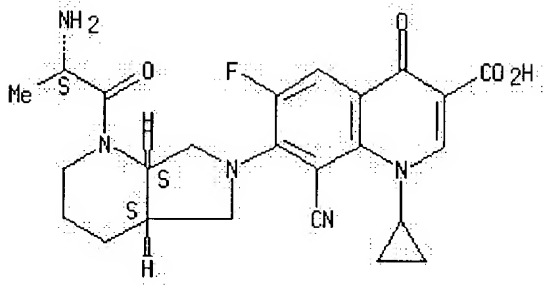
Absolute stereochemistry.



RN 195532-36-6 HCAPLUS
CN 3-Quinolinecarboxylic acid, 7-[1-(2-amino-1-oxopropyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, monohydrochloride, [4aS-[1(R*),4aα,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

h eb c g cg b cg eb

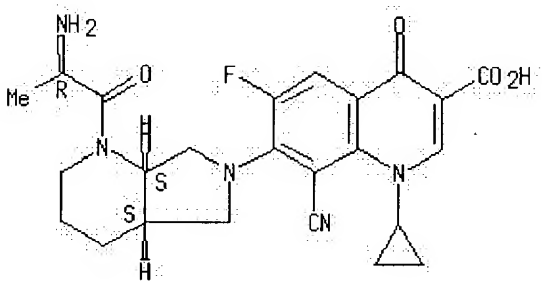


HCl

RN 195532-39-9 HCAPLUS

CN 3-Quinolinecarboxylic acid, 7-[1-(2-amino-1-oxopropyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, monohydrochloride, [4aS-[1(S*),4aα,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

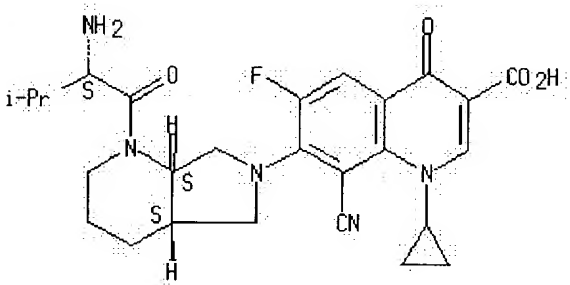


HCl

RN 195532-42-4 HCAPLUS

CN 3-Quinolinecarboxylic acid, 7-[1-(2-amino-3-methyl-1-oxobutyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, monohydrochloride, [4aS-[1(R*),4aα,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



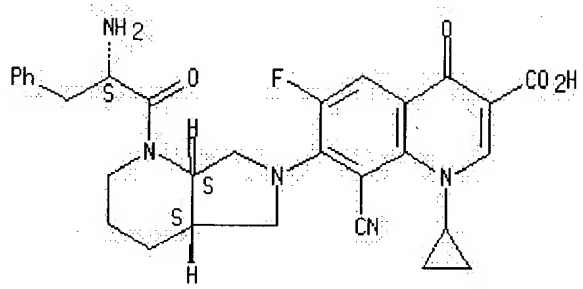
HCl

RN 195532-45-7 HCAPLUS

CN 3-Quinolinecarboxylic acid, 7-[1-(2-amino-1-oxo-3-phenylpropyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, monohydrochloride, [4aS-[1(R*),4aα,7aα]]- (9CI) (CA INDEX NAME)

h eb c g cg b cg eb

Absolute stereochemistry.

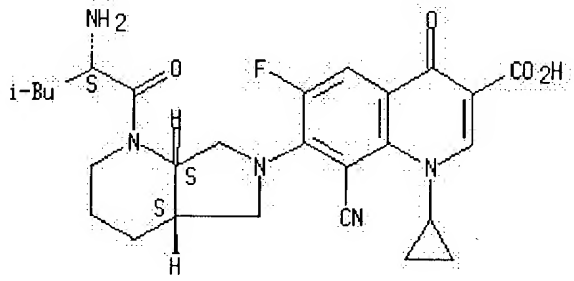


HCl

RN 195532-48-0 HCAPLUS

CN 3-Quinolinecarboxylic acid, 7-[1-(2-amino-4-methyl-1-oxopentyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-, monohydrochloride, [4aS-[1(R*),4aα,7aα]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

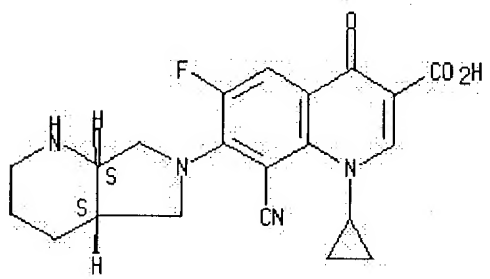


HCl

RN 195532-58-2 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monosodium salt, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



Na

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h . eb c g cg b cg eb

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    21.36     495.07

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -2.10      -2.10

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  assignees, and patent information, e.g., patent numbers, are
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  printed between 1907-1966 are available in the PAGE
  display formats.

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  more information.

=> d his

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L2            2 S L1
L3           23 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:58:20 ON 07 NOV 2004
L4           12 S L3

     FILE 'REGISTRY' ENTERED AT 22:58:25 ON 07 NOV 2004
L5              STRUCTURE UPLOADED
L6            0 S L5
L7           19 S L5 FULL

     FILE 'HCAPLUS' ENTERED AT 22:59:56 ON 07 NOV 2004
L8           31 S L7/RCT
L9            4 S L3/PREP
L10           3 S L9 AND L8

     FILE 'REGISTRY' ENTERED AT 23:00:15 ON 07 NOV 2004
L11             STRUCTURE UPLOADED
L12           4 S L11
L13          48 S L11 FULL

     FILE 'HCAPLUS' ENTERED AT 23:02:20 ON 07 NOV 2004
L14           8 S L13/RCT
L15           3 S L14 AND L10

     FILE 'CAOLD' ENTERED AT 23:04:14 ON 07 NOV 2004
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h eb c g cg b cg eb

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=> s L7 and L3
                1 L7
                0 L3
L16             0 L7 AND L3

=>
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h eb c g cg b cg eb

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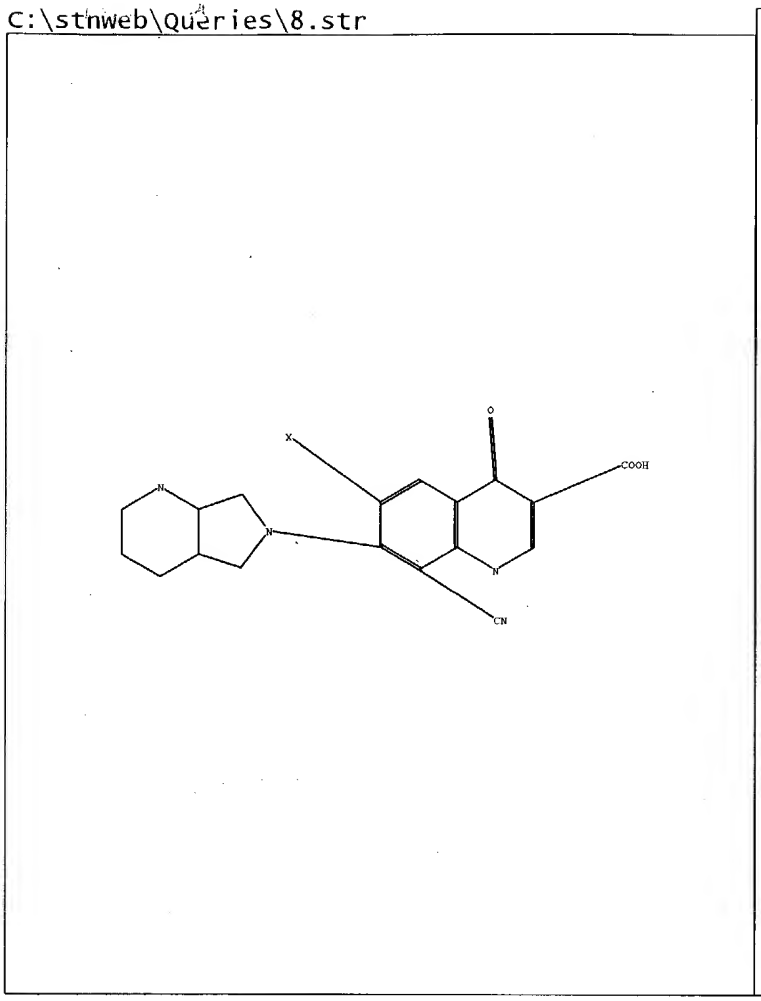

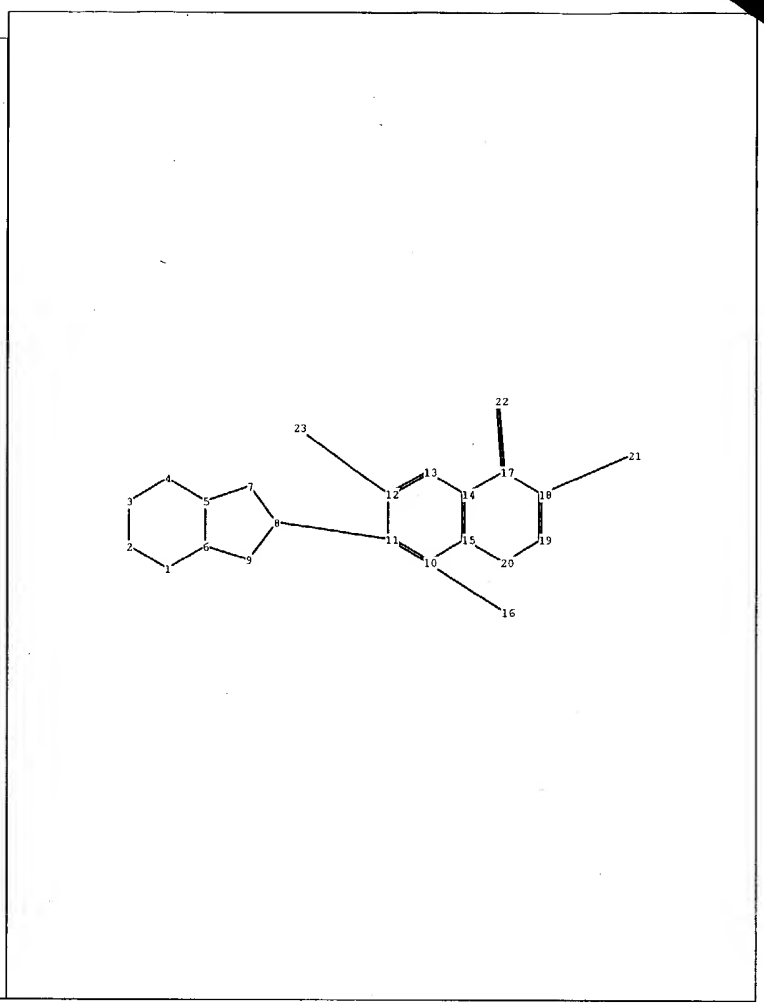

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16 21 22 23
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 17 18 19 20
chain bonds :
8-11 10-16 12-23 17-22 18-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15 14-17 15-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 8-11 14-17 15-20 17-18 17-22 18-19 19-20
exact bonds :
5-7 6-9 10-16 12-23 18-21
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 : 10 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
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21:CLASS 22:CLASS 23:CLASS

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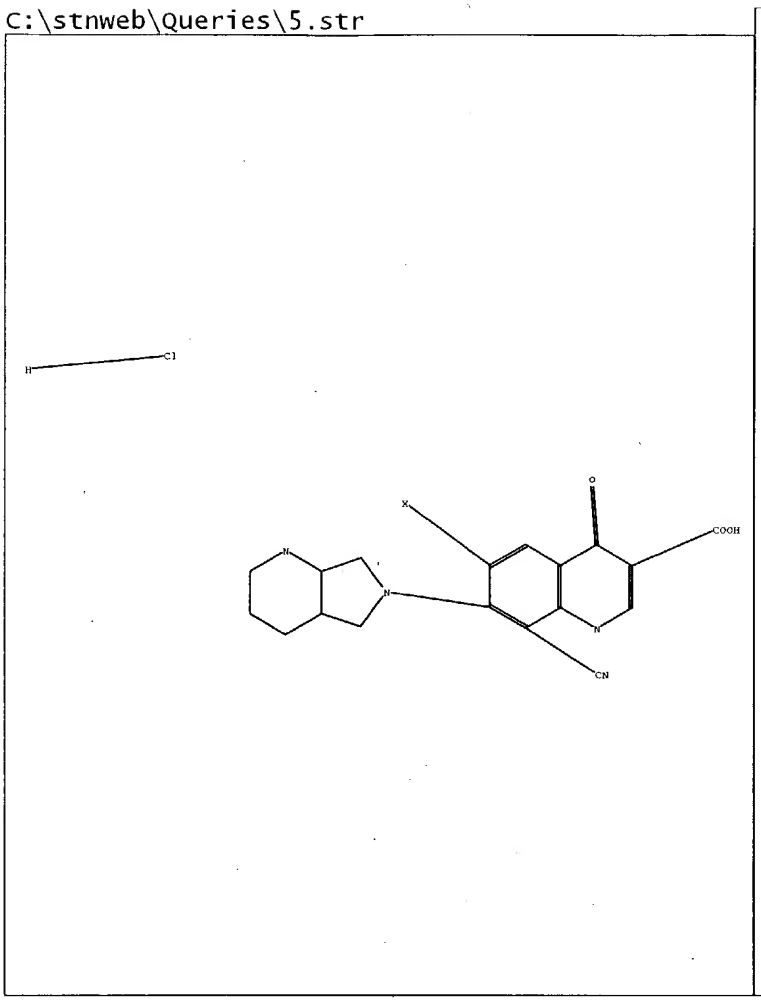

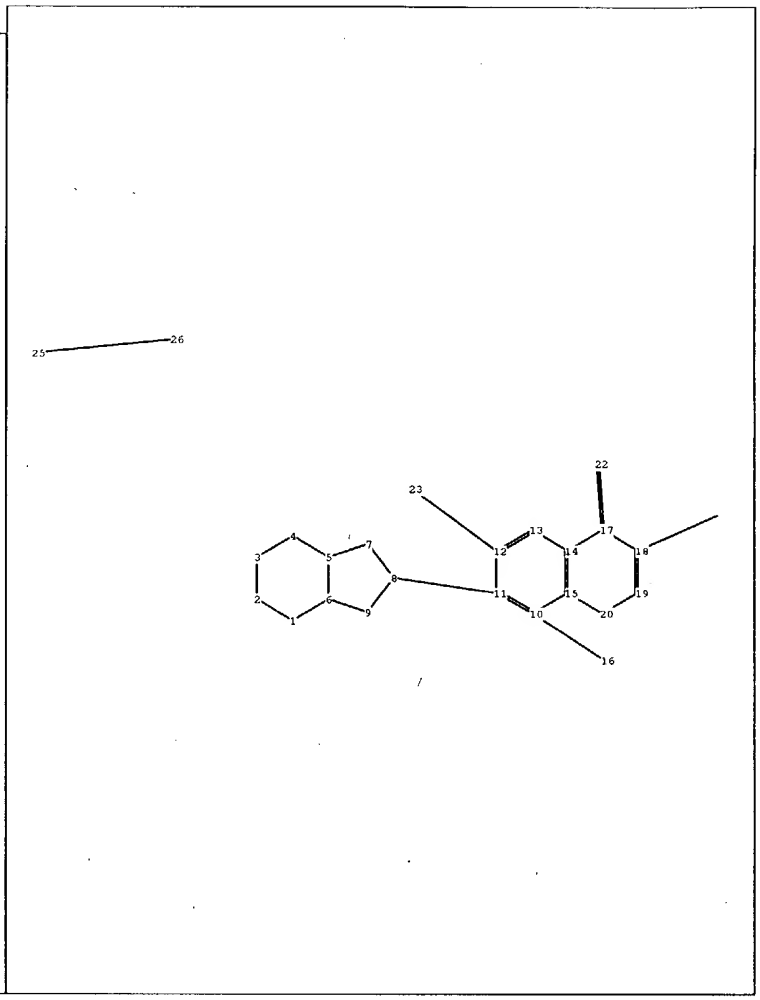

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ring nodes :
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chain bonds :
8-11 10-16 12-23 17-22 18-21 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15 14-17 15-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 8-11 14-17 15-20 17-18 17-22 18-19 19-20
exact bonds :
5-7 6-9 10-16 12-23 18-21 25-26
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 : 10 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom
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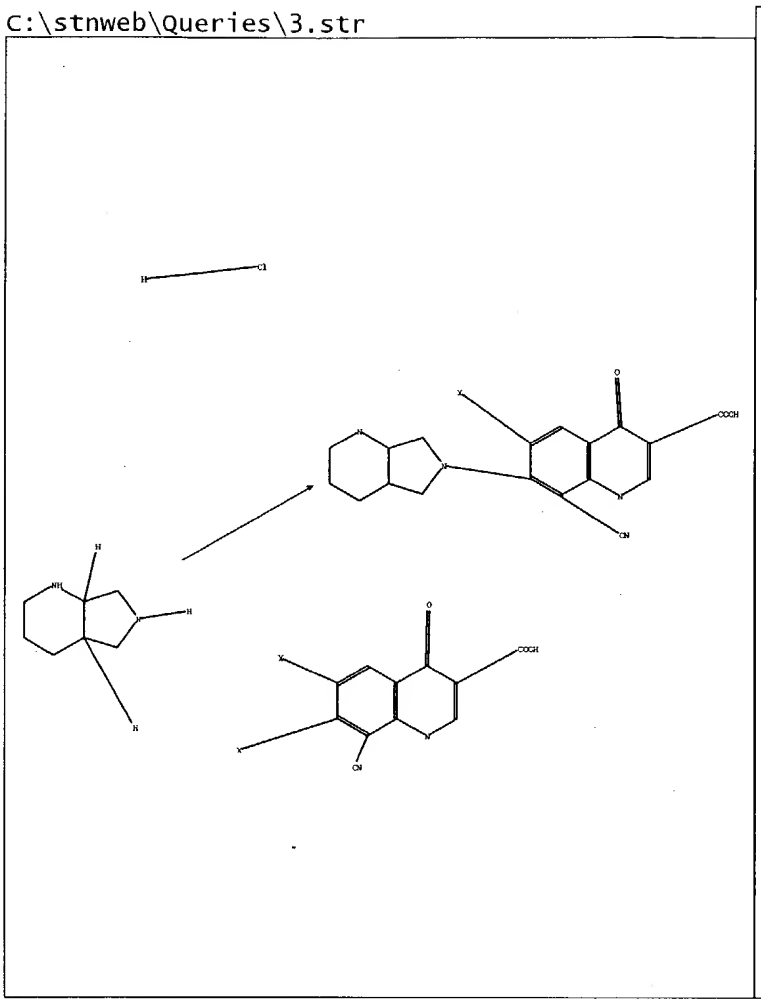

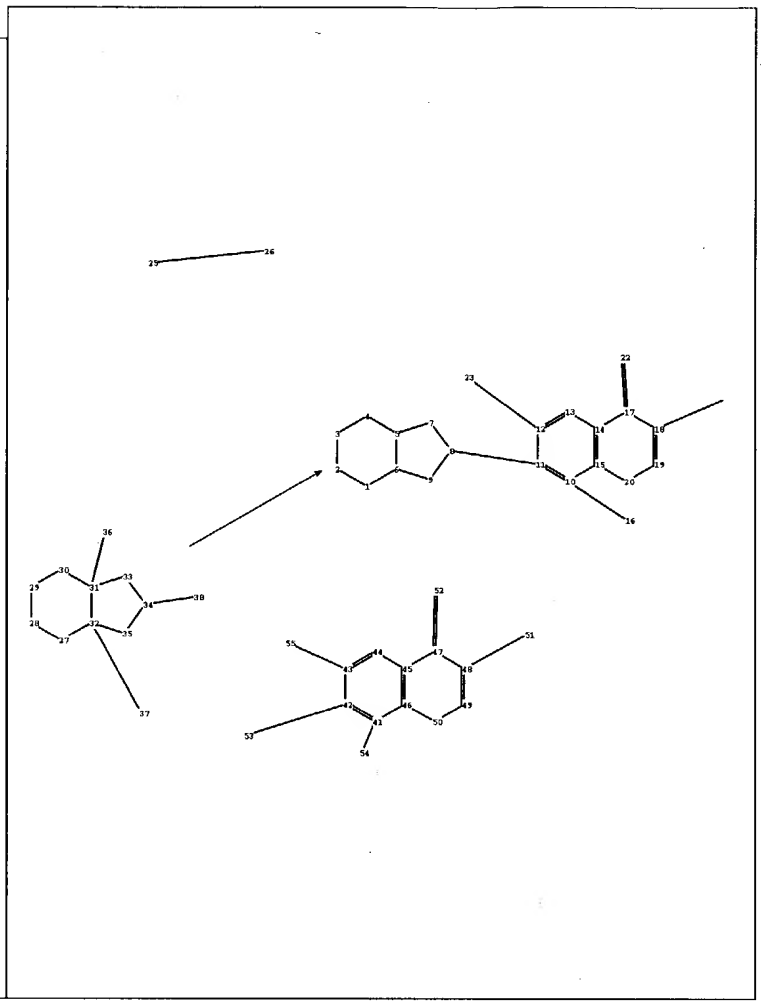

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ring nodes :
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33 34 35 41 42 43 44 45 46 47 48 49 50
chain bonds :
8-11 10-16 12-23 17-22 18-21 25-26 31-36 32-37 34-38 41-54 42-53 43-55 47-52
48-51
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15 14-17 15-20 17-18 18-19 19-20 27-28 27-32 28-29 29-30 30-31 31-32 31-33
32-35 33-34 34-35 41-42 41-46 42-43 43-44 44-45 45-46 45-47 46-50 47-48 48-49
49-50
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 8-11 14-17 15-20 17-18 17-22 18-19 19-20
27-28 27-32 28-29 29-30 30-31 31-32 33-34 34-35 45-47 46-50 47-48 47-52 48-49
49-50
exact bonds :
5-7 6-9 10-16 12-23 18-21 25-26 31-33 31-36 32-35 32-37 34-38 41-54 42-53
43-55 48-51
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15 41-42 41-46 42-43 43-44 44-45 45-46
isolated ring systems :
containing 1 : 10 : 27 : 41 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:CLASS 25:CLASS 26:CLASS 27:Atom 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS 38:CLASS 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:CLASS
52:CLASS 53:CLASS 54:CLASS 55:CLASS
fragments assigned reactant role:

containing 27
fragments assigned product role:
containing 1
containing 25

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* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1          Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2          "Ask CAS" for self-help around the clock
 NEWS  3  JUL 12  BEILSTEIN enhanced with new display and select options,
                  resulting in a closer connection to BABS
 NEWS  4  AUG 02  IFIPAT/IFIUDB/IFICDB reloaded with new search and display
                  fields
 NEWS  5  AUG 02  CAplus and CA patent records enhanced with European and Japan
                  Patent Office Classifications
 NEWS  6  AUG 02  The Analysis Edition of STN Express with Discover!
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                  status data from INPADOC
 NEWS  9  SEP 01  INPADOC: New family current-awareness alert (SDI) available
 NEWS 10  SEP 01  New pricing for the Save Answers for SciFinder Wizard within
                  STN Express with Discover!
 NEWS 11  SEP 01  New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
 NEWS 12  SEP 27  STANDARDS will no longer be available on STN
 NEWS 13  SEP 27  SWETSCAN will no longer be available on STN
 NEWS 14  OCT 28  KOREAPAT now available on STN

 NEWS EXPRESS  OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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 NEWS INTER    General Internet Information
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 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

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specific topic.

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FILE 'HOME' ENTERED AT 21:07:21 ON 07 NOV 2004

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.42       0.42

FILE 'REGISTRY' ENTERED AT 21:08:29 ON 07 NOV 2004
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provided by InfoChem.

STRUCTURE FILE UPDATES:     5 NOV 2004  HIGHEST RN 775356-23-5
DICTIONARY FILE UPDATES:    5 NOV 2004  HIGHEST RN 775356-23-5
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h eb c g cg b cg eb

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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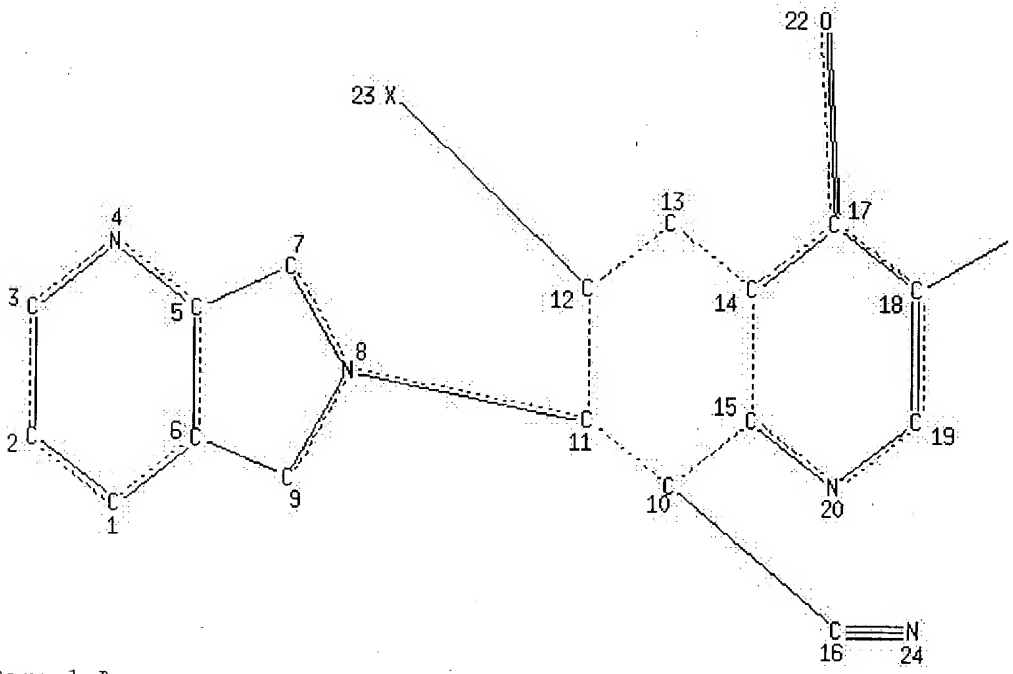
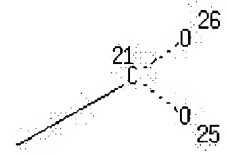
L1 HAS NO ANSWERS
L1 STR



Page 1-A



Page 1-B
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NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS R AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS R AT 10

h eb c g cg b cg eb

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NSPEC   IS R      AT  11
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NSPEC   IS R      AT  13
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NSPEC   IS R      AT  15
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NSPEC   IS C      AT  21
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NSPEC   IS C      AT  26
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MLEVEL  IS CLASS  AT  16 21 22 23 24 25 26
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  26

STEREO ATTRIBUTES: NONE


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SAMPLE SCREEN SEARCH COMPLETED -      6 TO ITERATE

100.0% PROCESSED       6 ITERATIONS                              2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            6 TO      266
PROJECTED ANSWERS:               2 TO      124

L2            2 SEA SSS SAM L1

=> s l1 full
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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:12:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     70 TO ITERATE

100.0% PROCESSED      70 ITERATIONS                             23 ANSWERS
SEARCH TIME: 00.00.01

L3           23 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               157.94     158.36

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 7 Nov 2004 VOL 141 ISS 20
FILE LAST UPDATED: 6 Nov 2004 (20041106/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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L4 12 L3

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61 HIMMLER, T?/AU
L5 6 L4 AND HIMMLER, T?/AU

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L5 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:607382 HCAPLUS
DOCUMENT NUMBER: 133:213147
TITLE: Crystal modification C of 8-cyano-1-cyclopropyl-7-[(1S,6S)-2,8-diazabicyclo[4.3.0]nonan-8-yl]-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): Rast, Hubert; **Himmler, Thomas**
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19908449	A1	20000831	DE 1999-19908449	19990226
CA 2362801	AA	20000908	CA 2000-2362801	20000214
WO 2000052009	A1	20000908	WO 2000-EP1202	20000214

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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JP 2002538158	T2	20021112	JP 2000-602235	20000214
AT 226952	E	20021115	AT 2000-909166	20000214
PT 1155018	T	20030228	PT 2000-909166	20000214
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NO 2001004061	A	20010821	NO 2001-4061	20010821
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			WO 2000-EP1202 W	20000214

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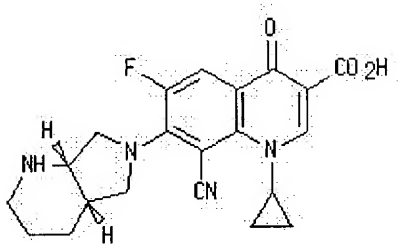


I

AB The title compd. (I) is converted to stable crystal modification C (m. 235-237°) by holding I at room temp. and relative humidity ≥92% until no further wt. gain occurs, drying, and heating to above the conversion temp. (150-180°). I modification D is characterized by its powder x-ray diffractogram, IR spectrum, and by DTA. I is highly active against pathogenic bacteria in human and veterinary medicine.

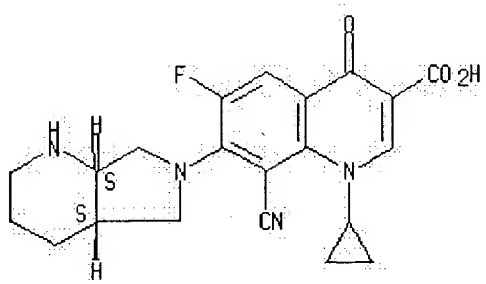
IT **195532-12-8**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(crystal modification D of cyanocyclopropyl(diazabicyclononanyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

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Full Text | Citing References

ACCESSION NUMBER: 2000:607381 HCAPLUS
DOCUMENT NUMBER: 133:213146
TITLE: Crystal modification D of 8-cyano-1-cyclopropyl-7-[(1S,6S)-2,8-diazabicyclo[4.3.0]nonan-8-yl]-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid

INVENTOR(S): **Himmler, Thomas**; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany

SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19908448	A1	20000831	DE 1999-19908448	19990226
CA 2362804	AA	20000908	CA 2000-2362804	20000214
WO 2000052010	A1	20000908	WO 2000-EP1203	20000214
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EP 1159277	A1	20011205	EP 2000-909167	20000214
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AU 760710	B2	20030522	AU 2000-31544	20000214
AU 2000031544	A5	20000921		
NZ 513749	A	20031031	NZ 2000-513749	20000214
ZA 2001006050	A	20020724	ZA 2001-6050	20010724
NO 2001004059	A	20010821	NO 2001-4059	20010821
US 6492391	B1	20021210	US 2001-914031	20010822

PRIORITY APPLN. INFO.: DE 1999-19908448 A 19990226
WO 2000-EP1203 W 20000214

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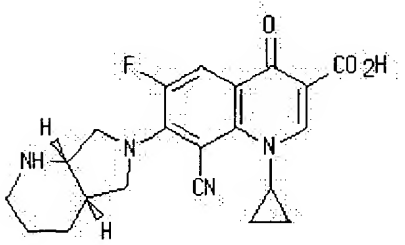

I

AB The title compd. (I) is converted to stable crystal modification D (m. 261-265°) by dissolving I in H2O to a concn. of 1-3 wt.%, allowing the soln. to stand until a ppt. forms, removing the ppt. by filtration, drying the remaining soln., and heating the solid obtained to above the

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transition temp. (130-160°). I modification D is characterized by its powder x-ray diffractogram, IR spectrum, and by DTA. I is highly active against pathogenic bacteria in human and veterinary medicine.

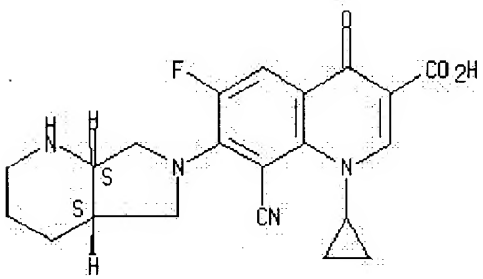
IT **195532-12-8**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(crystal modification D of cyanocyclopropyl(diazabicyclononanyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:366037 HCAPLUS
DOCUMENT NUMBER: 133:4647
TITLE: Semihydrochloride of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): **Himmler, Thomas**; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 16 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854357	A1	20000531	DE 1998-19854357	19981125
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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EP 1133495	A1	20010919	EP 1999-955995	19991115

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EP 1133495	B1	20021009			
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NO 2001002532	A	20010702	NO 2001-2532		20010523
PRIORITY APPLN. INFO.:			DE 1998-19854357	A	19981125
			WO 1999-EP8778	W	19991115

OTHER SOURCE(S): CASREACT 133:4647

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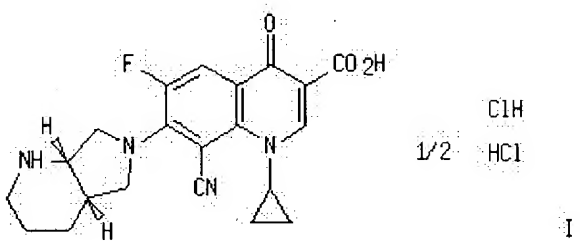


I

AB The title compd. (I), useful as a medical and veterinary bactericide, shows good water soly. (19 wt.%). I is produced by reaction of 7-halo-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid with (1S,6S)-2,8-diazabicyclo[4.3.0]nonane in the presence of a base in one of the following diluents: (a) a C≥4 aliph. alc., (b) a mixt. of a C>3 alc. with the polar aprotic diluent, N-methylpyrrolidone; (c) a mixt. of n-PrOH with DMF. I (m. 278-280°) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

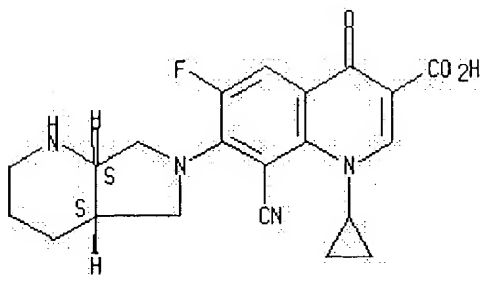
IT **271252-05-2P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(semihydrochloride of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 271252-05-2 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, hydrochloride (2:1) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



1/2 HCl

h eb c g cg b cg eb

L5 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2000:366036 HCAPLUS
DOCUMENT NUMBER: 133:4646
TITLE: Crystal modification A of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): **Himmler, Thomas**; Hallenbach, Werner; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854356	A1	20000531	DE 1998-19854356	19981125
CA 2351712	AA	20000602	CA 1999-2351712	19991115
WO 2000031075	A1	20000602	WO 1999-EP8775	19991115
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 9915669	A	20010814	BR 1999-15669	19991115
EP 1133496	A1	20010919	EP 1999-958040	19991115
EP 1133496	B1	20040421		
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TR 200101438	T2	20011022	TR 2001-200101438	19991115
JP 2002530406	T2	20020917	JP 2000-583903	19991115
NZ 511861	A	20021220	NZ 1999-511861	19991115
AU 763883	B2	20030731	AU 2000-15533	19991115
CN 1135229	B	20040121	CN 1999-813686	19991115
TW 576835	B	20040221	TW 1999-88119810	19991115
AT 264858	E	20040515	AT 1999-958040	19991115
PT 1133496	T	20040831	PT 1999-958040	19991115
NO 2001002460	A	20010518	NO 2001-2460	20010518
US 6436955	B1	20020820	US 2001-856669	20010523

PRIORITY APPLN. INFO.:

DE 1998-19854356	A	19981125
WO 1999-EP8775	W	19991115

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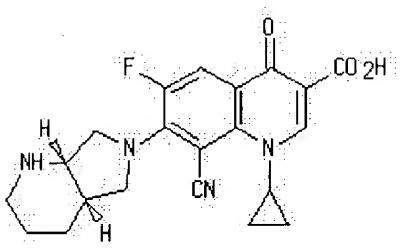


I

h eb c g cg b cg eb

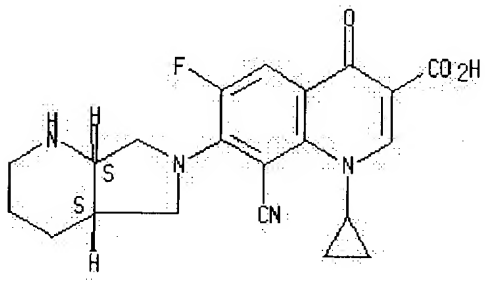
AB The title compd. in crystal modification A (I), useful as a medical and veterinary bactericide, is stable during extended storage without conversion to the amorphous form or any other crystal modification, and is less hygroscopic than the amorphous form of the compd. I is produced by dissolving the amorphous compd. or an unknown modification of it in hot water or a hot water-alc. mixt., adding an alc. (esp. EtOH or iso-PrOH), and cooling to room temp. I (m. 249-252°) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

IT **195532-12-8P**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystal modification A of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:366035 HCAPLUS
DOCUMENT NUMBER: 133:4645
TITLE: Crystal modification B of 8-cyano-1-cyclopropyl-7-(1S,6S-2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S): **Himmler, Thomas**; Hallenbach, Werner; Rast, Hubert
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854355	A1	20000531	DE 1998-19854355	19981125
CA 2351707	AA	20000602	CA 1999-2351707	19991115
WO 2000031076	A1	20000602	WO 1999-EP8776	19991115

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

h eb c g cg b cg eb

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

BR 9915682	A	20010814	BR 1999-15682		19991115
EP 1133497	A1	20010919	EP 1999-959278		19991115
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
TR 200101444	T2	20020121	TR 2001-200101444		19991115
JP 2002530407	T2	20020917	JP 2000-583904		19991115
NZ 511862	A	20030829	NZ 1999-511862		19991115
AU 767890	B2	20031127	AU 2000-16517		19991115
NO 2001002461	A	20010518	NO 2001-2461		20010518
US 6664268	B1	20031216	US 2001-856670		20010523
PRIORITY APPLN. INFO.:			DE 1998-19854355	A	19981125
			WO 1999-EP8776	W	19991115

OTHER SOURCE(S): CASREACT 133:4645

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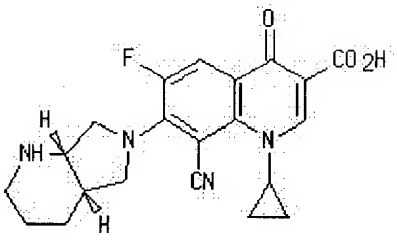


I

AB The title compd. in crystal modification B (I), useful as a medical and veterinary bactericide, is stable during extended storage without conversion to the amorphous form or any other crystal modification, and is less hygroscopic than the amorphous form of the compd. I is produced either (a) by reaction of 7-halo-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid with (1S,6S)-2,8-diazabicyclo[4.3.0]nonane in the presence of a base in a mixt. of EtOH and a polar aprotic diluent such as N-methylpyrrolidone, DMF, or sulfolane, or (b) by heating an unknown modification of the compd. in the presence of a base in EtOH, n-PrOH, iso-PrOH, or a mixt. of one of these alcs. with one of the polar aprotic diluents named previously. I (m. 243-245°) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

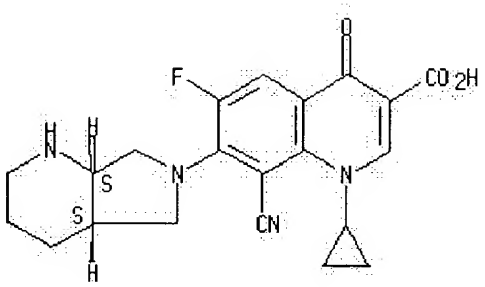
IT **195532-12-8P**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(crystal modification B of cyanocyclopropyl(diazabicyclononyl)fluorodihydrooxoquinolinecarboxylic acid)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | String References

ACCESSION NUMBER: 1997:579724 HCAPLUS
DOCUMENT NUMBER: 127:248093
TITLE: 8-Cyano-1-cyclopropyl-7-(2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid derivatives
INVENTOR(S): Bartel, Stefan; Jaetsch, Thomas; **Himmler, Thomas**; Rast, Hans-Georg; Hallenbach, Werner; Heinen, Ernst; Pirro, Franz; Scheer, Martin; Stegemann, Michael; Stupp, Hans-Peter; Wetzstein, Heinz-Georg
PATENT ASSIGNEE(S): Bayer A.-G., Germany; Bartel, Stefan; Jaetsch, Thomas; Himmler, Thomas; Rast, Hans-Georg; Hallenbach, Werner; Heinen, Ernst; Pirro, Franz; Scheer, Martin; et al.
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9731001	A1	19970828	WO 1997-EP637	19970212
W: AU, BB, BG, BR, BY, CA, CN, CZ, HU, IL, JP, KR, KZ, LK, MX, NO, NZ, PL, RO, RU, SK, TR, UA, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19633805	A1	19970828	DE 1996-19633805	19960822
ZA 9701507	A	19970916	ZA 1997-1507	19970202
CA 2247020	AA	19970828	CA 1997-2247020	19970212
AU 9717689	A1	19970910	AU 1997-17689	19970212
AU 715341	B2	20000120		
EP 882049	A1	19981209	EP 1997-903260	19970212
EP 882049	B1	20021120		
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CN 1211984	A	19990324	CN 1997-192523	19970212
CN 1073112	B	20011017		
BR 9707606	A	19990727	BR 1997-7606	19970212
NZ 331468	A	20000228	NZ 1997-331468	19970212
JP 2000504734	T2	20000418	JP 1997-529755	19970212
IL 125444	A1	20010319	IL 1997-125444	19970212
RU 2173318	C2	20010910	RU 1998-117814	19970212
EP 1215202	A1	20020619	EP 2002-6519	19970212
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AT 228130	E	20021215	AT 1997-903260	19970212
CZ 291251	B6	20030115	CZ 1998-2684	19970212
ES 2184060	T3	20030401	ES 1997-903260	19970212

h eb c g cg b cg eb

PT 882049	T	20030430	PT 1997-903260		19970212
PL 186737	B1	20040227	PL 1997-328577		19970212
TW 390879	B	20000521	TW 1997-86101994		19970220
US 6323213	B1	20011127	US 1998-125191		19980813
NO 9803819	A	19980820	NO 1998-3819		19980820
HK 1018903	A1	20020510	HK 1999-104030		19990917
US 6278013	B1	20010821	US 2000-718062		20001121
CN 1335301	A	20020213	CN 2001-110855		20010228
PRIORITY APPLN. INFO.:			DE 1996-19606762	A	19960223
			DE 1996-19633805	A	19960822
			EP 1997-903260	A3	19970212
			WO 1997-EP637	W	19970212
			US 1998-125191	A3	19980813

OTHER SOURCE(S): MARPAT 127:248093

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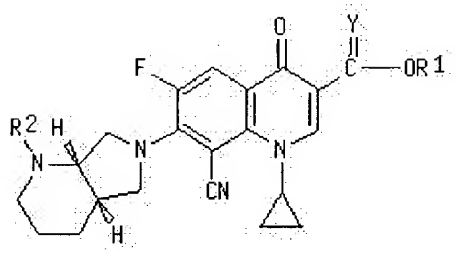


I

AB Title compds. I [R1 = H, alkyl, optionally substituted by OH, OMe, NH2, NHMe, NMe2, or (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl; R2 = H, benzyl, alkyl, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl, CH=CHCO2R3, CH2CH2CO2R3, CH2CH2CN, CH2CH2COMe, CH2COMe; R3 = Me, Et, R4(NHCHR5CO)n; R4 = H, alkyl, CO2CMe3; R5 = H, alkyl, hydroxyalkyl, aminoalkyl, thioalkyl, carboxyalkyl, benzyl; n = 1, 2; Y = O, S] were prepd. for use as antibacterial agents. Thus, I [R1 = OH, R2 = H, Y = O] was prepd. by aminating the 7-chloroquinoline. I [R1 = OH, R2 = H, Y = O] had min. inhibitory concns. against a no. of bacteria that were superior to those of enrofloxacin.

IT **195532-12-8P**

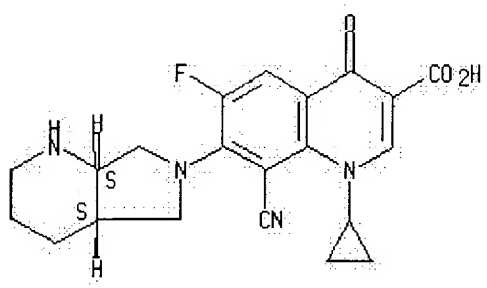
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of diazabicylononylquinolinecarboxylic acid derivs. as bactericides)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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=> d his

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L2              2 S L1
L3             23 S L1 FULL

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L4             12 S L3
L5              6 S L4 AND HIMMLER, T?/AU

=> s l4 not l5
L6              6 L4 NOT L5

=> s l6 and rast, r?/au
            10 RAST, R?/AU
L7              0 L6 AND RAST, R?/AU

=> d l6, ibib abs fhitstr, 1-6

L6   ANSWER 1 OF 6  HCAPLUS  COPYRIGHT 2004 ACS on STN
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Full Text | More References

```
ACCESSION NUMBER:         2004:800774  HCAPLUS
DOCUMENT NUMBER:          141:282840
TITLE:                    Controlled-release drug delivery system containing
                          saccharose acetate isobutyrate (SAIB)
INVENTOR(S):              Fraatz, Kristine; Mertin, Dirk; Heep, Iris
PATENT ASSIGNEE(S):       Bayer Healthcare AG, Germany
SOURCE:                   Ger. Offen., 8 pp.
                          CODEN: GWXXBX
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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     DE 10312346           A1    20040930    DE 2003-10312346        20030320
     WO 2004082658         A1    20040930    WO 2004-EP2318          20040306
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
PRIORITY APPLN. INFO.:                        DE 2003-10312346    A  20030320
AB   The invention concerns controlled-release drug delivery systems that
     include (a) a drug; (b) saccharose acetate isobutyrate (SAIB); (c)
     glycerinformal, isopropylidene glycerol or their mixt. as solvent.  A
     cosolvent can be added; they are selected from the group of ethanol,
     n-butanol and benzyl alc.  Thus a formulation contained (wt./wt.%): SAIB
```

h eb c g cg b cg eb

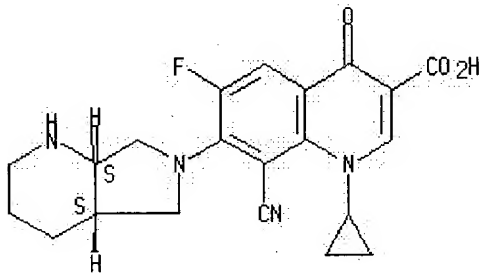
40; pradofloxacin 3; n-butanol 3; ethanol 5; 1N HCl 1.7; glycerinformal to 100.

IT **195532-12-8**, Pradofloxacin
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(controlled release drug delivery system contg. saccharose acetate isobutyrate (SAIB))

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2003:971863 HCAPLUS
DOCUMENT NUMBER: 140:31484
TITLE: Pharmaceutical preparations, especially quinolone antibiotics, for oral administration, containing ion-exchange resins loaded with active ingredients and intrinsically viscous gelling agents as thickening agents
INVENTOR(S): Mertin, Dirk; Edingloh, Markus; Daube, Gert
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003101422	A2	20031211	WO 2003-EP5228	20030519
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10224086	A1	20031211	DE 2002-10224086	20020531

PRIORITY APPLN. INFO.: DE 2002-10224086 A 20020531

AB The invention relates to pharmaceutical prepns. for oral administration,

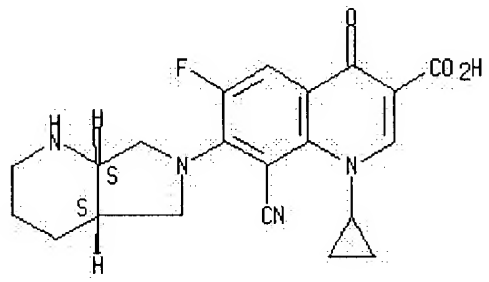
h eb c g cg b cg eb

said prepns. contg. at least one active ingredient which is bound to an ion exchanger. The inventive prepns. also contain an intrinsically viscous gelling agent as a thickening agent in order to improve their phys. stability and acceptance, esp. by animals. Thus 0.18 kg methyl-p-hydroxybenzoate and 0.02 kg propyl-p-hydroxybenzoate were dissolved in 75.0 kg hot water; 0.3 kg Xanthan gum and 0.3 kg bentonite were added under vigorous mixing; mixing was continued for one hour at 70°C. The mixt. was cooled; 6.0 kg pradofloxacin, 18.0 kG Amberlite IRP 64 and 1.0 kg vanillin were added to the sol.

IT **195532-12-8**, Pradofloxacin
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(pharmaceutical prepns., esp. quinolone antibiotics, for oral administration, contg. ion-exchange resins loaded with active ingredients and intrinsically viscous gelling agents as thickening agents)

RN 195532-12-8 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

ACCESSION NUMBER: 2003:744337 HCAPLUS
DOCUMENT NUMBER: 139:301379
TITLE: Clinical efficacy and safety of pradofloxacin in the treatment of canine pyoderma and wound infections under field conditions
AUTHOR(S): Stephan, B.; Hellmann, K.; Liege, P.; Granier, S.; Knoppe, T. N.; Heinen, E.; Greife, H. A.
CORPORATE SOURCE: Animal Health Business Group, Bayer AG, Leverkusen, Germany
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (2003), 26(Suppl. 1), 217-218
CODEN: JVPTD9; ISSN: 0140-7783
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Pradofloxacin is a novel 8-cyanofluoroquinolone with improved in vitro activity against a wide range of pathogenic bacteria. Tablets of different strengths are currently developed for the treatment of bacterial infections in dogs and cats. The objective of this work was to assess the clin. efficacy and safety of pradofloxacin in the treatment of canine pyoderma and wound infections.

IT **195532-12-8**, Pradofloxacin

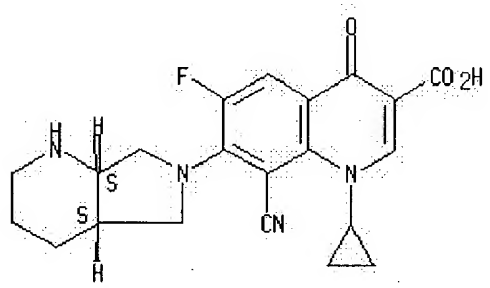
h eb c g cg b cg eb

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(clin. efficacy and safety of pradofloxacin in treatment of canine pyoderma and wound infections under field conditions)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Other References

ACCESSION NUMBER: 2003:744304 HCAPLUS
DOCUMENT NUMBER: 140:331682
TITLE: Analytical method for the determination of pradofloxacin in serum and urine by turbulent flow chromatography/tandem mass spectrometry
AUTHOR(S): Krebber, R.
CORPORATE SOURCE: Bayer CropScience AG, BCS-D-ROCS, Monheim, Germany
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (2003), 26(Suppl. 1), 102-103
CODEN: JVPTD9; ISSN: 0140-7783
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A high-throughput anal. method was developed and validated for the detn. of pradofloxacin (PRA) concns. in body fluids. A turbulent flow chromatog. system 2300 HTLC with auto injector CTC HTS PAL coupled to a tandem mass spectrometer Sciex API 365 was used. Serum and urine samples of dogs and cats were analyzed within a mean accuracy between -1 and 4% and a precision between 5.1 and 7.8%. The method enables direct anal. of PRA in several body fluids. It combines a min. of sample prepn. with fast and highly selective detn. within an extremely wide range of linearity and is therefore highly suitable to assess PRA concns. in pharmacokinetic studies.

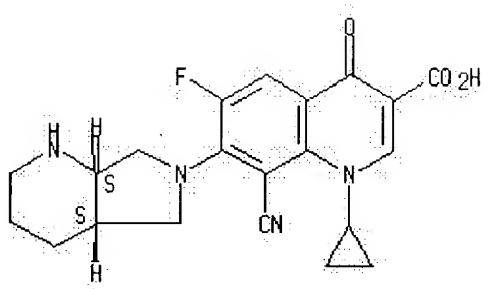
IT **195532-12-8**, Pradofloxacin
RL: ANT (Analyte); ANST (Analytical study)
(anal. method for detn. of pradofloxacin in serum and urine by turbulent flow chromatog./tandem mass spectrometry in cats and dogs)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

h eb c g cg b cg eb



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:744303 HCAPLUS
DOCUMENT NUMBER: 140:331734
TITLE: Protein binding of pradofloxacin, a novel 8-cyanofluoroquinolone, in dog and cat plasma
AUTHOR(S): Bregante, M. A.; De Jong, A.; Calvo, A.; Hernandez, E.; Rey, R.; Garcia, M. A.
CORPORATE SOURCE: Veterinary Faculty of University of Zaragoza, Zaragoza, Spain
SOURCE: Journal of Veterinary Pharmacology and Therapeutics (2003), 26(Suppl. 1), 87-88
CODEN: JVPTD9; ISSN: 0140-7783
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

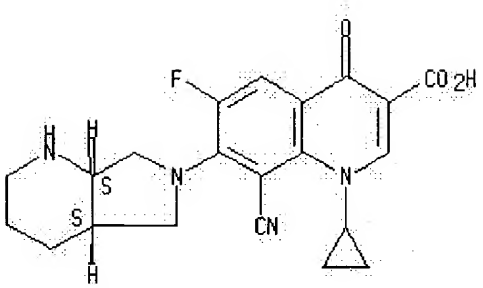
AB The in vitro protein binding of pradofloxacin (PRA) in plasma of dogs and cats was investigated. Enrofloxacin (ENR), the first veterinary fluoroquinolone, was tested as a ref. drug. For concns. of 0.15, 0.75 and 1.50 μg/mL, the percentages of free unbound drug in dog plasma were 63.4±14.8, 63.6±10.5 and 64.2±8.8 for PRA and 59.7±13.3, 54.3±7.3 and 68.4±5.0 for ENR, resp. In cat plasma, the percentages unbound drug were 68.6±7.8, 70.4±11.5, and 71.2±6.2 for PRA and 63.7±10.5, 66.0±9.8 and 73.4±12.5 for ENR. The plasma protein binding of PRA amounted to 29-37% over a ten-fold concn. range: similar findings for ENR (27-46% bound) are in agreement with previous results. A concn. dependency was absent for PRA, but in case of ENR there were statistically significant differences both in dogs and cats; the numerical differences, however, were small.

IT **195532-12-8**, Pradofloxacin
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(protein binding of pradofloxacin, novel 8-cyanofluoroquinolone, in dog and cat plasma)

RN 195532-12-8 HCAPLUS
CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

h eb c g cg b cg eb



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text | More References

ACCESSION NUMBER: 2003:76654 HCAPLUS
DOCUMENT NUMBER: 138:126984
TITLE: Pharmaceutical preparations for oral administration containing ion exchange resins loaded with active ingredients
INVENTOR(S): Mertin, Dirk; Block, Wolfgang; Hamann, Hans-juergen
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003007995	A2	20030130	WO 2002-EP7417	20020704
WO 2003007995	A3	20030731		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10134719	A1	20030206	DE 2001-10134719	20010717
EP 1411894	A2	20040428	EP 2002-743262	20020704
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002011149	A	20040629	BR 2002-11149	20020704

PRIORITY APPLN. INFO.:

DE 2001-10134719	A	20010717
WO 2002-EP7417	W	20020704

AB The invention relates to pharmaceutical prepns. contg. at least one active ingredient which is linked to an ion exchanger. In order to improve the palatability and to increase the stability, at least 90 % of said active ingredient/ion exchanger particles are smaller than 50 μm. Quinolone antibiotics are bound to cation exchange resins, esp. for the prepn. cat medication. Thus 3.86 kg enrofloxacin and 19.24 kg Amberlite IRP64 were suspended in 76.90 kg purified water and stirred for at least 8 h at room temp. The suspension was transferred to a filter dryer, filtered and dryed at 85°C. The obtained 17.96 kg of enrofloxacin-loaded resin

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was suspended with 60 g colloidal silica, 100.30 kg neutral oil (e.g. Miglyol 812) and ground in a perl mill; at least 90% of the particles were smaller than 10 μm.

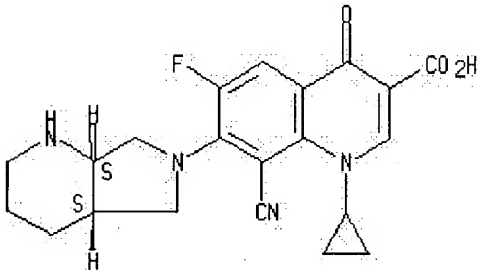
IT **195532-12-8**

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical prepns. for oral administration contg. ion exchange resins loaded with active ingredients)

RN 195532-12-8 HCAPLUS

CN 3-Quinolinecarboxylic acid, 8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	68.92	227.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-8.40	-8.40

FILE 'CAOLD' ENTERED AT 21:15:21 ON 07 NOV 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGistRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 21:07:21 ON 07 NOV 2004)

FILE 'REGISTRY' ENTERED AT 21:08:29 ON 07 NOV 2004
L1 STRUCTURE UPLOADED

h eb c g cg b cg eb

```
L2             2 S L1
L3            23 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 21:12:24 ON 07 NOV 2004
L4            12 S L3
L5             6 S L4 AND HIMMLER, T?/AU
L6             6 S L4 NOT L5
L7             0 S L6 AND RAST, R?/AU

     FILE 'CAOLD' ENTERED AT 21:15:21 ON 07 NOV 2004

=> s l3
L8             0 L3

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY     SESSION
FULL ESTIMATED COST                                    0.42      227.70

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                      ENTRY     SESSION
CA SUBSCRIBER PRICE                                    0.00       -8.40

FILE 'REGISTRY' ENTERED AT 21:15:28 ON 07 NOV 2004
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STRUCTURE FILE UPDATES:    5 NOV 2004  HIGHEST RN 775356-23-5
DICTIONARY FILE UPDATES:   5 NOV 2004  HIGHEST RN 775356-23-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L9       STRUCTURE UPLOADED

=> d l9
L9 HAS NO ANSWERS
L9              STR

=> s l9
SAMPLE SEARCH INITIATED 21:20:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      6 TO ITERATE

100.0% PROCESSED       6 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01
```

h ebc gcgb cg eb

```
FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:             6 TO      266
PROJECTED ANSWERS:                0 TO        0

L10           0 SEA SSS SAM L9

=> s l9 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:20:27 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      70 TO ITERATE

100.0% PROCESSED      70 ITERATIONS                              0 ANSWERS
SEARCH TIME: 00.00.01

L11           0 SEA SSS FUL L9

=>
L12     STRUCTURE UPLOADED

=> file casreact
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     173.06     400.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)            SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -8.40

FILE 'CASREACT' ENTERED AT 21:41:29 ON 07 NOV 2004
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26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 7 Nov 2004 VOL 141 ISS 19

************************************************************
*                                                          *
*     CASREACT now has more than  8 million reactions      *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.

=>
L13     STRUCTURE UPLOADED

=> d l13
L13 HAS NO ANSWERS
L13             STR
```

h eb c g cg b cg eb

```
=> s l13
SAMPLE SEARCH INITIATED 21:41:51 FILE 'CASREACT'
SCREENING COMPLETE -      0 REACTIONS TO VERIFY FROM      0 DOCUMENTS

100.0% DONE      0 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:         0 TO        0
PROJECTED ANSWERS:               0 TO        0

L14           0 SEA SSS SAM L13 (     0 REACTIONS)

=> s l13 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 21:41:56 FILE 'CASREACT'
SCREENING COMPLETE -      1 REACTIONS TO VERIFY FROM      1 DOCUMENTS

100.0% DONE      1 VERIFIED       1 HIT RXNS                      1 DOCS
SEARCH TIME: 00.00.01

L15           1 SEA SSS FUL L13 (     1 REACTIONS)

=> d l15, ibib abs crc, 1
'CRC' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
```

h eb c g cg b cg eb

```
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>).  Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD.  The information is displayed in the same order
as the specification.  All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

     (FILE 'HOME' ENTERED AT 21:07:21 ON 07 NOV 2004)

     FILE 'REGISTRY' ENTERED AT 21:08:29 ON 07 NOV 2004
L1              STRUCTURE UPLOADED
L2            2 S L1
L3           23 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 21:12:24 ON 07 NOV 2004
L4           12 S L3
L5            6 S L4 AND HIMMLER, T?/AU
L6            6 S L4 NOT L5
L7            0 S L6 AND RAST, R?/AU

     FILE 'CAOLD' ENTERED AT 21:15:21 ON 07 NOV 2004
L8            0 S L3
```

h eb c g cg b cg eb

```
     FILE 'REGISTRY' ENTERED AT 21:15:28 ON 07 NOV 2004
L9                STRUCTURE UPLOADED
L10           0 S L9
L11           0 S L9 FULL
L12               STRUCTURE UPLOADED

     FILE 'CASREACT' ENTERED AT 21:41:29 ON 07 NOV 2004
L13               STRUCTURE UPLOADED
L14           0 S L13
L15           1 S L13 FULL

=> d l15, ibib abs crd, 1


L15  ANSWER 1 OF 1  CASREACT  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

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ACCESSION NUMBER:         133:4647  CASREACT
TITLE:                    Semihydrochloride of 8-cyano-1-cyclopropyl-7-(1S,6S-
                          2,8-diazabicyclo[4.3.0]nonan-8-yl)-6-fluoro-1,4-
                          dihydro-4-oxo-3-quinolinecarboxylic acid
INVENTOR(S):              Himmler, Thomas; Rast, Hubert
PATENT ASSIGNEE(S):       Bayer A.-G., Germany
SOURCE:                   Ger. Offen., 16 pp.
                          CODEN: GWXXBX
DOCUMENT TYPE:            Patent
LANGUAGE:                 German
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19854357	A1	20000531	DE 1998-19854357	19981125
CA 2351714	AA	20000602	CA 1999-2351714	19991115
WO 2000031077	A1	20000602	WO 1999-EP8778	19991115
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
BR 9915684	A	20010814	BR 1999-15684	19991115
EP 1133495	A1	20010919	EP 1999-955995	19991115
EP 1133495	B1	20021009		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200101443	T2	20010921	TR 2001-20010144319991115	
JP 2002530408	T2	20020917	JP 2000-583905	19991115
AT 225790	E	20021015	AT 1999-955995	19991115
ES 2181488	T3	20030216	ES 1999-955995	19991115
PT 1133495	T	20030228	PT 1999-955995	19991115
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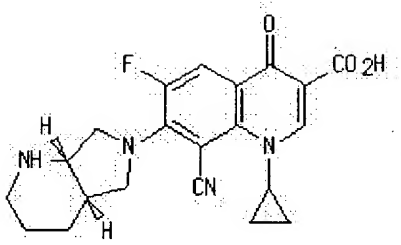
NZ 511863	A	20030530	NZ 1999-511863	19991115
NO 2001002532	A	20010702	NO 2001-2532	20010523
PRIORITY APPLN. INFO.:			DE 1998-19854357	19981125
			WO 1999-EP8778	19991115

h eb c g cg b cg eb

GI

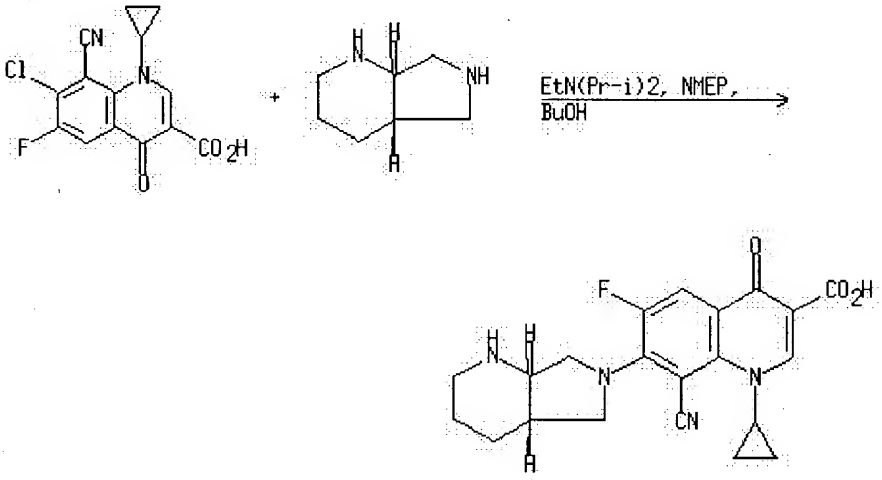


1/2 ClH HCl

I

AB The title compd. (I), useful as a medical and veterinary bactericide, shows good water soly. (19 wt.%). I is produced by reaction of 7-halo-8-cyano-1-cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid with (1S,6S)-2,8-diazabicyclo[4.3.0]nonane in the presence of a base in one of the following diluents: (a) a C≥4 aliph. alc., (b) a mixt. of a C>3 alc. with the polar aprotic diluent, N-methylpyrrolidone; (c) a mixt. of n-PrOH with DMF. I (m. 278-280°) is characterized by its powder x-ray diffractogram, differential thermogram, and IR spectrum.

RX(1) OF 1

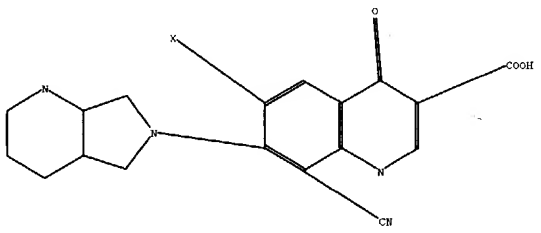


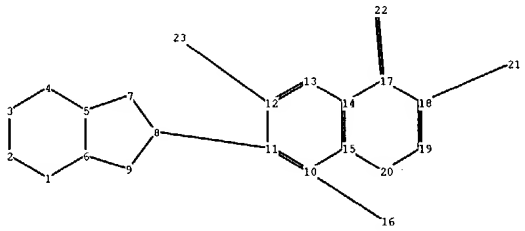
1/2 HCl

=>

h eb c g cg b cg eb

C:\stnweb\Queries\4.str

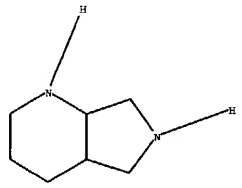


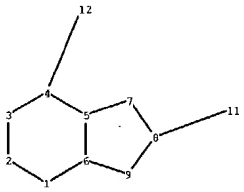


chain nodes :
16 21 22 23
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 17 18 19 20
chain bonds :
8-11 10-16 12-23 17-22 18-21
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 10-11 10-15 11-12 12-13 13-14
14-15 14-17 15-20 17-18 18-19 19-20
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 8-11 14-17 15-20 17-18 17-22 18-19 19-20
exact bonds :
5-7 6-9 10-16 12-23 18-21
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 : 10 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom 18:Atom 19:Atom 20:Atom
21:CLASS 22:CLASS 23:CLASS

C:\stnweb\Queries\4a.str





```
chain nodes :
    11  12
ring nodes :
    1  2  3  4  5  6  7  8  9
chain bonds :
    4-12  8-11
ring bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  7-8  8-9
exact bonds :
    4-12  5-7  6-9  8-11
isolated ring systems :
    containing 1 :


Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  11:CLASS
    12:CLASS
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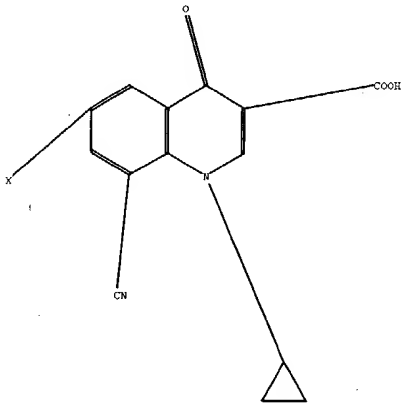
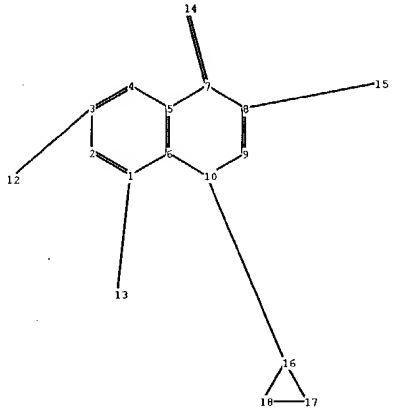
C:\stnweb\Queries\4a.str





chain nodes :
12 13 14 15
ring nodes :
1 2 3 4 5 6 7 8 9 10 16 17 18
chain bonds :
1-13 3-12 7-14 8-15 10-16
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-18 17-18
exact/norm bonds :
5-7 6-10 7-8 7-14 8-9 9-10 10-16 16-17 16-18 17-18
exact bonds :
1-13 3-12 8-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS
13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom

```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS   1            Web Page URLs for STN Seminar Schedule - N. America
 NEWS   2            "Ask CAS" for self-help around the clock
 NEWS   3  JUL 12    BEILSTEIN enhanced with new display and select options,
                     resulting in a closer connection to BABS
 NEWS   4  AUG 02    IFIPAT/IFIUDB/IFICDB reloaded with new search and display
                     fields
 NEWS   5  AUG 02    CAplus and CA patent records enhanced with European and Japan
                     Patent Office Classifications
 NEWS   6  AUG 02    The Analysis Edition of STN Express with Discover!
                     (Version 7.01 for Windows) now available
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 NEWS   8  AUG 27    BIOTECHABS/BIOTECHDS: Two new display fields added for legal
                     status data from INPADOC
 NEWS   9  SEP 01    INPADOC: New family current-awareness alert (SDI) available
 NEWS  10  SEP 01    New pricing for the Save Answers for SciFinder Wizard within
                     STN Express with Discover!
 NEWS  11  SEP 01    New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
 NEWS  12  SEP 27    STANDARDS will no longer be available on STN
 NEWS  13  SEP 27    SWETSCAN will no longer be available on STN
 NEWS  14  OCT 28    KOREAPAT now available on STN

 NEWS EXPRESS  OCTOBER 29 CURRENT WINDOWS VERSION IS V7.01A, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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 NEWS INTER    General Internet Information
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 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
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FILE 'HOME' ENTERED AT 22:56:26 ON 07 NOV 2004

=> file reg
COST IN U.S. DOLLARS                                  SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

FILE 'REGISTRY' ENTERED AT 22:56:32 ON 07 NOV 2004
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STRUCTURE FILE UPDATES:     5 NOV 2004  HIGHEST RN 775356-23-5
DICTIONARY FILE UPDATES:    5 NOV 2004  HIGHEST RN 775356-23-5
```

h eb c g cg b cg eb

```
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1      STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 22:58:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      6 TO ITERATE

100.0% PROCESSED       6 ITERATIONS                              2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            6 TO      266
PROJECTED ANSWERS:               2 TO      124

L2            2 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 22:58:18 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     70 TO ITERATE

100.0% PROCESSED      70 ITERATIONS                             23 ANSWERS
SEARCH TIME: 00.00.01

L3            23 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               156.26     156.47

FILE 'HCAPLUS' ENTERED AT 22:58:20 ON 07 NOV 2004
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```

h eb c g cg b cg eb

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FILE COVERS 1907 - 7 Nov 2004 VOL 141 ISS 20
FILE LAST UPDATED: 6 Nov 2004 (20041106/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 22:56:26 ON 07 NOV 2004)

FILE 'REGISTRY' ENTERED AT 22:56:32 ON 07 NOV 2004
L1 STRUCTURE UPLOADED
L2 2 S L1
L3 23 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:58:20 ON 07 NOV 2004

=> s l3
L4 12 L3

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 2.36 158.83

FILE 'REGISTRY' ENTERED AT 22:58:25 ON 07 NOV 2004
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STRUCTURE FILE UPDATES: 5 NOV 2004 HIGHEST RN 775356-23-5
DICTIONARY FILE UPDATES: 5 NOV 2004 HIGHEST RN 775356-23-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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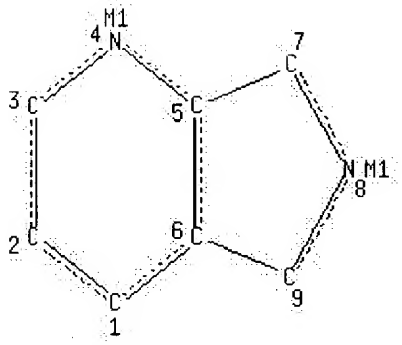
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR

h eb c g cg b cg eb




```
NODE ATTRIBUTES:
HCOUNT   IS M1      AT    4
HCOUNT   IS M1      AT    8
NSPEC    IS R       AT    1
NSPEC    IS R       AT    2
NSPEC    IS R       AT    3
NSPEC    IS R       AT    4
NSPEC    IS R       AT    5
NSPEC    IS R       AT    6
NSPEC    IS R       AT    7
NSPEC    IS R       AT    8
NSPEC    IS R       AT    9
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS   9

STEREO ATTRIBUTES: NONE


=> s l5
SAMPLE SEARCH INITIATED 22:59:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   7119 TO ITERATE

 14.0% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       137323 TO   147437
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5

=> s l5 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 22:59:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 142269 TO ITERATE

100.0% PROCESSED  142269 ITERATIONS                              19 ANSWERS
SEARCH TIME: 00.00.01

L7           19 SEA SSS FUL L5
```

h eb c g cg b cg eb

```
=> file hcaplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       156.26     315.09

FILE 'HCAPLUS' ENTERED AT 22:59:56 ON 07 NOV 2004
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FILE LAST UPDATED: 6 Nov 2004  (20041106/ED)

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 substance identification.


=> s l7/rct
           36 L7
      2674061 RCT/RL
L8         31 L7/RCT
                (L7 (L) RCT/RL)

=> d his

     (FILE 'HOME' ENTERED AT 22:56:26 ON 07 NOV 2004)

     FILE 'REGISTRY' ENTERED AT 22:56:32 ON 07 NOV 2004
L1               STRUCTURE UPLOADED
L2            2 S L1
L3           23 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:58:20 ON 07 NOV 2004
L4           12 S L3

     FILE 'REGISTRY' ENTERED AT 22:58:25 ON 07 NOV 2004
L5               STRUCTURE UPLOADED
L6            0 S L5
L7           19 S L5 FULL

     FILE 'HCAPLUS' ENTERED AT 22:59:56 ON 07 NOV 2004
L8           31 S L7/RCT

=> s l3/prep
           12 L3
      3219792 PREP/RL
L9         4 L3/PREP
                (L3 (L) PREP/RL)
```

h eb c g cg b cg eb